

A Unified Theory of Quantum Holonomies

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Abstract

A periodic change of slow environmental parameters of a quantum system induces quantum holonomy. The phase holonomy is a well-known example. Another is a more exotic kind that exhibits eigenvalue and eigenspace holonomies. We introduce a theoretical formulation that describes the phase and eigenspace holonomies on an equal footing. The key concept of the theory is a gauge connection for an ordered basis, which is conceptually distinct from Mead-Truhlar-Berry's connection and its Wilczek-Zee extension. A gauge invariant treatment of eigenspace holonomy based on Fujikawa's formalism is developed. Example of adiabatic quantum holonomy, including the exotic kind with spectral degeneracy, are shown.

Key words: geometric phase, exotic holonomies, gauge theory

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1. Introduction

Consider a quantum system in a stationary state. Let us adiabatically change a parameter of the system along a closed path where the spectral degeneracy is assumed to be absent. We ask the destination of the state after a change of the parameter along the path. This question is frequently raised in discussions of the Berry phase [1]. An answer, which is widely shared since Berry's work, is that a discrepancy remains in the phase of the state vector, even after the dynamical phase is excluded. Indeed this is correct in a huge amount of examples [2, 3]. However, it is shown that this answer is not universal in a recent report of exotic anholonomies [4] in which the initial and the final states are orthogonal in spite of the absence of the spectral degeneracy. In other words, the eigenspace associated with the adiabatic cyclic evolution exhibits discrepancy, or anholonomy. Furthermore, the eigenspace discrepancy induces another discrepancy in the corresponding eigenenergy.

For the phase discrepancy, an established interpretation in terms of differential geometry allows us to call it the phase *holonomy* [5]. This interpretation naturally invites its non-Abelian extension, which has been subsequently discovered by Wilczek and Zee in systems with spectral degeneracies [6]. Contrary to this, any successful association of the eigenspace discrepancy with the concept of holonomy has not been known.

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The aim of this paper is to demonstrate that an interpretation of the eigenspace discrepancy in terms of holonomy is indeed possible. To achieve this, we introduce a framework that treats the phase and the eigenspace holonomies in a unified manner in Section 2. The key concept is a non-Abelian gauge connection that is associated with a parameterized basis [7], and the identification of the place where the gauge connection resides in the time evolution. This is achieved through a fully gauge invariant extension of Fujikawa's formulation that has been introduced for the phase holonomy [8, 9]. Our approach is illustrated by the analysis of adiabatic quantum holonomies of three examples. First, Berry's Hamiltonian with spin- $\frac{1}{2}$ is revisited in Section 3. The role of parallel transport [10, 5], which accompanies the multiple-valuedness of a parameterized basis, in our formulation will be emphasized. The second example, shown in Section 4, exhibits exotic holonomies without spectral degeneracy. The last example, shown in Section 5, is the simplest examples of the exotic holonomies in the presence of degeneracy, i.e., the eigenspace holonomy á la Wilczek and Zee. Section 6 provides a summary and an outlook. A brief, partial report of the present result can be found in Ref. [11].

2. A gauge theory for a parameterized basis

Two building blocks of our theory, a gauge connection that is associated with a parameterized basis [7], and Fujikawa formalism, originally conceived for the phase holonomy, are presented in order to introduce our approach to quantum holonomies.

2.1. A gauge connection

In the presence of the quantum holonomy, basis vectors are, in general, multiple-valued as functions of a parameter. In order to cope with such multiple-valuedness, we introduce a gauge connection for a parameterized basis. This has been introduced by Filipp and Sjöqvist [7] to examine Manini-Pistolesi off-diagonal geometric phase [12]. As is explained below, this gauge connection is different from Mead-Truhlar-Berry's [13, 1] and Wilczek-Zee's gauge connections [6], which describe solely the phase holonomy.

For N -dimensional Hilbert space \mathcal{H} , let $\{|\xi_n(s)\rangle\}_{n=0}^{N-1}$ be a complete orthogonal normalized system that is smoothly depends on a parameter s . The parametric dependence induces a gauge connection $A(s)$, which is a $N \times N$ Hermite matrix and whose (n, m) -th element is

$$A_{nm}(s) \equiv i\langle \xi_n(s) | \frac{\partial}{\partial s} | \xi_m(s) \rangle. \quad (1)$$

By definition, $A(s)$ is non-Abelian. For given $A(s)$, the basis vector $|\xi_n(s)\rangle$ obeys the following differential equation

$$i \frac{\partial}{\partial s} |\xi_m(s)\rangle = \sum_n A_{nm}(s) |\xi_n(s)\rangle \quad (2)$$

and we may solve this equation with an "initial condition" at $s = s'$.

The dynamical variable of the equation of motion (2) is an ordered sequence of basis vectors, also called a frame,

$$f(s) \equiv [|\xi_0(s)\rangle, |\xi_1(s)\rangle, \dots, |\xi_{N-1}(s)\rangle]. \quad (3)$$

Its conjugation

$$f(s)^\dagger = \begin{bmatrix} \langle \xi_0(s) | \\ \langle \xi_1(s) | \\ \vdots \\ \langle \xi_{N-1}(s) | \end{bmatrix} \quad (4)$$

is also useful. For example, the resolution of unity by $\{|\xi_n(s)\rangle\}_{n=0}^{N-1}$ is expressed as

$$f(s) \{f(s)^\dagger\} = \hat{1}_{\mathcal{H}}, \quad (5)$$

where $\hat{1}_{\mathcal{H}}$ is the identical operator for \mathcal{H} , and the gauge connection $A(s)$ is written as

$$A(s) = i \{f(s)^\dagger\} \frac{\partial}{\partial s} f(s). \quad (6)$$

Now we have the equation of motion for $f(s)$

$$i \frac{\partial}{\partial s} f(s) = f(s) A(s). \quad (7)$$

Its formal solution is

$$f(s'') = f(s') \exp_{\rightarrow} \left(-i \int_{s'}^{s''} A(s) ds \right), \quad (8)$$

where \exp_{\rightarrow} is the anti-ordered exponential for the contour integration by s [7]. Note that we need to specify the integration path to deal with the multiple-valuedness of $f(s)$, in general.

Our designation “gauge connection” for the whole $A(s)$ is intended to clarify the difference from two famous gauge connections for the phase holonomy. When we choose $\{|\xi_n(s)\rangle\}_{n=0}^{N-1}$ as an adiabatic basis of a non-degenerate Hamiltonian $\hat{H}(s)$ with an adiabatic parameter s , the elements of the gauge connection $A(s)$ have a well-known interpretation: A diagonal element $A_{nn}(s)$ is Mead-Truhlar-Berry’s Abelian gauge connection for a single adiabatic state $|\xi_n(s)\rangle$. The off-diagonal elements are nonadiabatic transition matrix elements, and, constitute “the field strength” corresponding to Mead-Truhlar-Berry’s Abelian gauge connection [1]. This also applies to a degenerate Hamiltonian with Wilczek-Zee’s non-Abelian gauge connection, which describes the change in an eigenspace. On the other hand, $A(s)$ that contains all elements $\{A_{mn}(s)\}$ is defined with respect to the change of the frame $f(s)$, instead of each eigenspace [7]. As to be shown below, $A(s)$ plays the central role in the quantum holonomy.

2.2. An extended Fujikawa formalism

Fujikawa has introduced a formulation to examine the quantum holonomy accompanying time evolution that involves a change of a parameter [8, 9]. We will focus on the unitary time evolution for pure state in the following. As a building block of the time evolution, we examine a parameterized quantum map, whose stroboscopic, unit time evolution from $|\psi'\rangle$ to $|\psi''\rangle$ is described by

$$|\psi''\rangle = \hat{U}(s) |\psi'\rangle, \quad (9)$$

where $\hat{U}(s)$ is a unitary operator with a parameter s . This is because periodically driven systems, whose Floquet operator is $\hat{U}(s)$, are our primary examples, and our approach is immediately

applicable to a Hamiltonian time evolution, where $\hat{U}(s)$ correspond to an infinitesimal time evolution operator. Let us vary s along a path C in the parameter space during L iterations of the quantum map (9), where s' and s'' is the initial and final points, respectively. Accordingly we examine the whole time evolution operator

$$\hat{U}(\{s_l\}_{l=0}^{L-1}) \equiv \hat{U}(s_{L-1})\hat{U}(s_{L-2}) \cdots \hat{U}(s_0), \quad (10)$$

where s_l is the value of s at l -th step. Although the present formulation is applicable to investigate nonadiabatic settings, our primary interest here is an adiabatic behavior induced by the limiting procedure $L \rightarrow \infty$. The “ $f(s)$ -representation” of the building block $\hat{U}(s)$ of the whole evolution is a $N \times N$ unitary matrix

$$Z(s) \equiv \{f(s)^\dagger\} \hat{U}(s) f(s). \quad (11)$$

In other words, we have $\hat{U}(s) = f(s)Z(s)\{f(s)^\dagger\}$. In order to deal with the change of s from s_l to s_{l+1} , we have

$$\begin{aligned} \hat{U}(s_l) &= f(s_{l+1})\{f(s_{l+1})^\dagger\} \times \hat{U}(s_l) \\ &= f(s_{l+1})Z_F(s_{l+1}, s_l)\{f(s_l)^\dagger\}, \end{aligned} \quad (12)$$

where an effective time evolution matrix $Z_F(s_{l+1}, s_l)$ incorporates the unit dynamical evolution and the parametric change of s along a part of path C

$$Z_F(s_{l+1}, s_l) \equiv \exp\left(i \int_{s_l}^{s_{l+1}} A(s) ds\right) Z(s_l), \quad (13)$$

where \exp_{\leftarrow} is the ordered exponential. Hence the whole time evolution is expressed as

$$\hat{U}(\{s_l\}_{l=0}^{L-1}) = f(s'')B_d(\{s_l\}_{l=0}^L)\{f(s')^\dagger\} \quad (14)$$

where we have an “effective” time evolution operator

$$B_d(\{s_l\}_{l=0}^L) \equiv Z_F(s_L, s_{L-1})Z_F(s_{L-1}, s_{L-2}) \cdots Z_F(s_1, s_0). \quad (15)$$

Finally, we have “the $f(s')$ -representation” of the whole time evolution operator

$$\hat{U}(\{s_l\}_{l=0}^{L-1}) = f(s')W(C)B_d(\{s_l\}_{l=0}^L)\{f(s')^\dagger\}, \quad (16)$$

where

$$W(C) \equiv \exp\left(-i \int_C A(s) ds\right). \quad (17)$$

Since the above definitions are exact, our formulation is invariant against a basis transformation with $N \times N$ unitary matrix $G(s)$

$$f(s) \mapsto f(s)G(s) \quad (18)$$

once we incorporate the following transformations

$$A(s) \mapsto G(s)^\dagger A(s) G(s) + iG(s)^\dagger \frac{\partial G(s)}{\partial s}, \quad (19a)$$

$$W(C) \mapsto G(s')^\dagger W(C) G(s''), \quad (19b)$$

$$B_d(\{s_l\}_{l=0}^L) \mapsto G(s'')^\dagger B_d(\{s_l\}_{l=0}^L) G(s'). \quad (19c)$$

This is Fujikawa's hidden local gauge invariance [9] in a generalized form. The strategy of Fujikawa formalism is to extract a geometric information from the whole time evolution operator via the expression (16) with an appropriate restriction of $G(s)$, as is shown below.

Let us examine the case that the change of s is slow enough so that we may employ the adiabatic approximation [14]. Accordingly it is suitable to choose $f(s)$ as an adiabatic basis, i.e., each basis vector $|\xi_n(s)\rangle$ is an eigenvector of $\hat{U}(s)$, to make $Z(s)$ a diagonal matrix, whose non-zero elements are the eigenvalues of $\hat{U}(s)$. Let $z_n(s)$ be the eigenvalue of $\hat{U}(s)$ corresponding to an eigenvector $|\xi_n(s)\rangle$, i.e.,

$$\hat{U}(s)|\xi_n(s)\rangle = z_n(s)|\xi_n(s)\rangle, \quad (20)$$

where we assume that there is no degeneracy in eigenvalue. Note that $z_n(s)$ is unimodular due to the unitarity of $\hat{U}(s)$. Now the gauge transformation $G(s)$ is restricted to $U(1)^{\otimes N}$ times a permutation matrix, which correspond to the freedoms to choose the phases of basis vectors, and assign the quantum numbers, respectively. The permutation matrix is required to deal with the eigenspace holonomy, as is shown below. In terms of $Z_F(s_{l+1}, s_l)$, the adiabatic approximation is the diagonal approximation [9]

$$Z_F(s_{l+1}, s_l) \simeq Z_F^D(s_{l+1}, s_l) \equiv \exp \left(i \int_{s_l}^{s_{l+1}} A^D(s) ds \right) Z(s_l), \quad (21)$$

where $A^D(s)$ is the diagonal part of the gauge connection $A(s)$, i.e., $A_{mn}^D(s) = \delta_{mn} A_{mn}(s)$. Namely, $A_{mn}^D(s)$ is Mead-Truhlar-Berry's gauge connection for the m -th state $|\xi_m(s)\rangle$ [13, 1]. The corresponding adiabatic approximation of $B_d(\{s_l\}_{l=0}^L)$ (15) is

$$B_{ad}(\{s_l\}_{l=0}^L) \equiv Z_F^D(s_L, s_{L-1}) Z_F^D(s_{L-1}, s_{L-2}) \dots Z_F^D(s_1, s_0), \quad (22)$$

which are decomposed into two parts:

$$B_{ad}(\{s_l\}_{l=0}^L) = B(C) D(\{s_l\}_{l=0}^L), \quad (23a)$$

where

$$B(C) \equiv \exp \left(i \int_C A^D(s) ds \right) \quad (23b)$$

is the geometric part, and,

$$D(\{s_l\}_{l=0}^L) \equiv \prod_{l=0}^{L-1} Z(s_l) \quad (23c)$$

contains dynamical phases. We retain the path-ordered exponential in $B(C)$ to make it applicable to the cases with the presence of spectral degeneracies, as shown below. To sum up, the adiabatic approximation of the whole time evolution is

$$\hat{U}(\{s_l\}_{l=0}^{L-1}) \simeq f(s') M(C) D(\{s_l\}_{l=0}^L) \{f(s')^\dagger\}, \quad (24)$$

where

$$\begin{aligned} M(C) &\equiv W(C) B(C) \\ &= \exp_{\rightarrow} \left(-i \int_C A(s) ds \right) \exp_{\leftarrow} \left(i \int_C A^D(s) ds \right), \end{aligned} \quad (25)$$

is the geometric part determined by the path C , and two gauge connections $A(s)$ and $A^D(s)$.

For a cyclic path C , we call $M(C)$ (Eq. (25)) a *holonomy matrix*, which describes the adiabatic change of state vector, starting from an eigenstate at $s = s'$, along the closed path C .

An explanation why $W(C)$ is required to describe the eigenspace holonomy is the following. Let us assume that $f(s)$ is single-valued. This implies that $W(C)$ is the $N \times N$ identical matrix. Consequently, $M(C) = B(C)$ is always diagonal and thus cannot describe the eigenspace holonomy, though the single-valuedness assumption does not prevent the conventional approach from describing the phase holonomy. On the other hand, in the presence of the eigenspace holonomy, a factor of $M(C)$ need to be a permutation matrix. Since $B(C)$, which is always a diagonal matrix according to its definition, cannot be such a factor, the permutation matrix is need to be supplied by $W(C)$. This is consistent with the fact that the presence of the eigenspace anholonomy implies the multiple-valuedness of $f(s)$.

Furthermore, when we employ the parallel transport condition $A^D(s) = 0$ [10, 5, 7], the holonomy matrix takes extremely simple form:

$$M^{\text{p.t.}}(C) = \exp_{\rightarrow} \left(-i \int_C A(s) ds \right), \quad (26)$$

which is determined only by $W(C)$. In other words, all the adiabatic quantum holonomies can be summarized as a holonomy in the ordered basis $f(s)$ (Eq. (3)). For the phase holonomy, this observation is already reported by Fujikawa [8, 9]. In this sense, the parallel transport condition offers a privileged gauge.

We explain the consequence of the gauge transformation (18) under the adiabatic approximation, where $G(s)$ is restricted to be a product of a permutation matrix and a diagonal unitary matrix. The invariance of the adiabatic time evolution operator, which appears at the right hand side of Eq. (24), is assured due to the following

$$A^D(s) \mapsto G(s)^\dagger A^D(s) G(s) + i G(s)^\dagger \frac{\partial G(s)}{\partial s}, \quad (27a)$$

$$W(C) \mapsto G(s')^\dagger W(C) G(s''), \quad (27b)$$

$$B(C) \mapsto G(s'')^\dagger B(C) G(s'). \quad (27c)$$

Hence we obtain the manifest covariance of $M(C)$

$$M(C) \mapsto G(s')^\dagger M(C) G(s'). \quad (28)$$

Eq. (25) provides a correct expression of the holonomy matrix $M(C)$ not only for maps (9) but also for flows, i.e., Hamiltonian systems and periodically driven systems. For a system whose time evolution is generated by a nearly static Hamiltonian $\hat{H}(s)$, we will derive Eq. (25) in Appendix A with a suitable discretization of time. For a periodically driven system described by a Hamiltonian $\hat{H}(t, s)$, where $\hat{H}(t, s) = \hat{H}(t + T, s)$ is assumed, a Floquet operator

$$\exp\left(-\frac{i}{\hbar} \int_0^T \hat{H}(t, s) dt\right) \quad (29)$$

is the unitary operator $\hat{U}(s)$ to provide a stroboscopic description of the system. Hence this system is reduced to a quantum map.

An extension of our formulation to the case that the presence of spectrum degeneracy whose degree is independent with s along a closed path C is shown. The resultant expression for the holonomy matrix (25) remains the same. This is achieved by a suitable extension of gauge connections $A(s)$ and $A^D(s)$. For the eigenspace corresponding to the eigenvalue $z_n(s)$ of $\hat{U}(s)$, we have a normalized orthogonal vectors $|\xi_{nv}(s)\rangle$ with an index v for the eigenspace, where

$$\hat{U}(s)|\xi_{nv}(s)\rangle = z_n(s)|\xi_{nv}(s)\rangle \quad (30)$$

and $\langle \xi_{n''v''}(s) | \xi_{n'v'}(s) \rangle = \delta_{n''n'} \delta_{v''v'}$. The gauge connection for the parameterized basis is

$$A_{n''v'', n'v'}(s) \equiv i \langle \xi_{n''v''}(s) | \frac{\partial}{\partial s} | \xi_{n'v'}(s) \rangle. \quad (31)$$

It is straightforward to see that $A^D(s)$ that appears in Eq. (25) is non-Abelian:

$$A_{n''v'', n'v'}^D(s) \equiv \delta_{n''n'} A_{n''v'', n'v'}(s), \quad (32)$$

where $A_{nv'}^D(s)$ is Wilcek-Zee's gauge connection for the n -th eigenspace [6].

3. An example of the phase holonomy

Our formulation is applied to Berry's simplest example of the adiabatic phase holonomy [1]. Let us suppose that a spin- $\frac{1}{2}$ is under static magnetic field \mathbf{B} . With a suitable choice of units, the spin is described by a Hamiltonian

$$\hat{H}(\mathbf{B}) = \mathbf{B} \cdot \hat{\boldsymbol{\sigma}}, \quad (33)$$

where $\hat{\boldsymbol{\sigma}} = \sum_{j=x,y,z} \hat{\sigma}_j \mathbf{e}_j$ is the Pauli operator for the spin, and, \mathbf{e}_j ($j = x, y, z$) is the unit vector for j -axis. The spectrum of $\hat{H}(\mathbf{B})$ is $\{\pm B\}$, where $B \equiv \|\mathbf{B}\|$. To investigate the adiabatic holonomy, we have to exclude the degeneracy point $B = 0$. The unit vector $\mathbf{n} \equiv \mathbf{B}/B$ is parameterized with the spherical coordinate, i.e., $\mathbf{n} = \mathbf{e}_x \cos \varphi \sin \theta + \mathbf{e}_y \sin \varphi \sin \theta + \mathbf{e}_z \cos \theta$. Let $|\xi_{\pm}(\mathbf{B})\rangle$ be a normalized eigenvector of $\hat{H}(\mathbf{B})$, corresponding to the eigenvalue $\pm B$:

$$|\xi_+(\mathbf{B})\rangle = e^{-i\varphi/2} \cos \frac{\theta}{2} |\uparrow\rangle + e^{i\varphi/2} \sin \frac{\theta}{2} |\downarrow\rangle \quad (34a)$$

$$|\xi_-(\mathbf{B})\rangle = -e^{-i\varphi/2} \sin \frac{\theta}{2} |\uparrow\rangle + e^{i\varphi/2} \cos \frac{\theta}{2} |\downarrow\rangle. \quad (34b)$$

Note that $|\xi_{\pm}(\mathbf{B})\rangle$ are multiple-valued as functions of (θ, φ) . To assure them single-valued, the range of (θ, φ) needs to be restricted within an open set $U_M \equiv \{(\theta, \varphi) | 0 < \theta < \pi \text{ and } 0 < \varphi < 2\pi\}$, for example. The corresponding frame $f(\mathbf{B}) \equiv [|\xi_+(\mathbf{B})\rangle, |\xi_-(\mathbf{B})\rangle]$ is

$$f(\mathbf{B}) = \begin{bmatrix} |\uparrow\rangle, & |\downarrow\rangle \end{bmatrix} \begin{bmatrix} e^{-i\varphi/2} \cos \frac{\theta}{2} & -e^{-i\varphi/2} \sin \frac{\theta}{2} \\ e^{i\varphi/2} \sin \frac{\theta}{2} & e^{i\varphi/2} \cos \frac{\theta}{2} \end{bmatrix}. \quad (35)$$

Gauge connections $A_x(\mathbf{B}) \equiv i\{f(\mathbf{B})^\dagger\} \partial f(\mathbf{B}) / \partial x$ ($x = \theta, \varphi, B$) for parametric changes of \mathbf{B} are

$$A_\theta(\mathbf{B}) = \frac{1}{2} \sigma_y, \quad (36a)$$

$$A_\varphi(\mathbf{B}) = \frac{1}{2} (\sigma_z \cos \theta - \sigma_x \sin \theta), \quad (36b)$$

$$A_B(\mathbf{B}) = 0, \quad (36c)$$

where we employ 2×2 complex matrices

$$\sigma_x \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (37)$$

Accordingly, the Mead-Truhlar-Berry gauge connections are

$$A_\theta^D(\mathbf{B}) = 0, \quad A_\varphi^D(\mathbf{B}) = \frac{1}{2} \sigma_z \cos \theta, \quad A_B^D(\mathbf{B}) = 0. \quad (38)$$

As is well known, the strength of the magnetic field B plays no particular role in the computation of the phase holonomy once B is kept nonzero.

Evaluations of the holonomy matrix $M(C)$ for typical closed loops in the parameter space are shown. First, we examine a loop C in which $f(\mathbf{B})$ is single-valued, e.g. $C \subset U_M$. Consequently $W(C)$ is the 2×2 identical matrix. This is a conventional wisdom to obtain a formula of the phase holonomy, where an appropriate gauge for $f(\mathbf{B})$ (or, equivalently, $|\xi_{\pm}(\mathbf{B})\rangle$) against the loop is chosen to avoid the multiple-valuedness of $f(\mathbf{B})$ [1]. Hence all the holonomies reside in $B(C) = M(C)$. The evaluation of the contour integral in $B(C)$ is straightforward to obtain the classic result in the matrix $M(C)$:

$$M(C) = \exp\left(-\frac{i}{2} \Omega(C) \sigma_z\right), \quad (39)$$

where $\Omega(C)$ is the solid angle for C [1].

Second, we examine a meridian great circle C_θ in which θ moves 0 to 2π with φ kept fixed. The parametric change along such a circle can induce a change of the sign of an eigenvector [15]. In our example, $f(\mathbf{B})$ cannot be single-valued on C_θ :

$$f(\mathbf{B})|_{\theta \downarrow 0} = -f(\mathbf{B})|_{\theta \uparrow 2\pi}. \quad (40)$$

Although the conventional strategy mentioned above is to avoid such multi-valuedness, we insist the present choice of the gauge (35) to show an alternative way to reproduce the conventional result. Thanks to the present choice of the gauge, the Mead-Truhlar-Berry gauge connection

satisfies the parallel transport condition $A_\theta^D = 0$ and $B(C_\theta) = 1$. This enable us to employ Eq. (26) to obtain the holonomy matrix:

$$M(C_\theta) = \exp \left(-i \oint_{C_\theta} \frac{1}{2} \sigma_y d\theta \right) = e^{-i\pi\sigma_y} = -1, \quad (41)$$

which is consistent with Eq. (39). This is an example that our formulation properly deals the multiple-valuedness of $f(\mathbf{B})$. On the other hand, if we choose an appropriate gauge to make $f(\mathbf{B})$ single-valued on the circuit C_θ , $W(C_\theta)$ is trivial to put all the nontrivial holonomy in $B(C_\theta)$, as is stated above.

Finally, let us consider a circle of latitude C_φ , where θ is kept fixed and φ is increased from 0 to 2π . It is straightforward to obtain $B(C_\varphi) = \exp(i\pi\sigma_z \cos \theta)$ and $W(C_\varphi) = -1$. The latter indicates again the sign change in the parametric dependence along C_φ . These elements are combined to reproduce a well-known result

$$M(C_\varphi) = \exp \{ -i\pi(1 - \cos \theta)\sigma_z \}. \quad (42)$$

We remark that, in all the examples above, the holonomy matrices M are diagonal, so that the eigenspace holonomy is absent. Accordingly the eigenvalue anholonomy is also absent.

4. An example of the exotic holonomies in quantum map spin- $\frac{1}{2}$

In Berry's Hamiltonian (Eq. (33)), the strength of the magnetic field B plays no role in quantum holonomies. One reason is that the corresponding gauge connection $A_B(\mathbf{B})$ vanishes. Another reason is that it is impossible to make any loop in the parameter space by an increment of B , with \mathbf{n} being kept fixed. To make a loop for a strength parameter, we may examine the following quantum map for a spin- $\frac{1}{2}$

$$\exp \{ -i\lambda (a + b\mathbf{n} \cdot \hat{\sigma}) \}, \quad (43)$$

where \mathbf{n} is a normalized real vector, a and b are real constants to be specified later, and λ is the strength. The periodicity of the quantum map with respect to the increment of λ implies that there is a loop in the parameter space of λ . In particular, if we choose $a = q/2$ and $b = (2 - q/2)$ with an integer q , Eq. (43) is periodic as a function of λ , with a primitive period 2π . Accordingly, the parameter space of λ is identified with S^1 and it might be suitable to investigate quantum holonomies for a periodic variation of λ . However, such a loop does not allow us to study adiabatic holonomies, since there remains a spectral degeneracy along the loop at $\lambda = 0 \pmod{2\pi}$.

A simple way to lift the degeneracy at $\lambda = 0$ is to concatenate two quantum maps:

$$\exp \left\{ -i\mu \left(\frac{q}{2} + \frac{2-q}{2} \mathbf{m} \cdot \hat{\sigma} \right) \right\} \exp \left\{ -i\lambda \left(\frac{p}{2} + \frac{2-p}{2} \mathbf{n} \cdot \hat{\sigma} \right) \right\}, \quad (44)$$

where q and p are integers, \mathbf{m} and \mathbf{n} are normalized vectors in \mathbb{R}^3 , and, μ and λ are strengths. Due to the periodicity in μ and λ , the parameter space of (μ, λ) is a two-dimensional torus $S^1 \times S^1$. Both \mathbf{m} and \mathbf{n} specify points on a sphere S^2 . In the following, we fix $\mathbf{m} = \mathbf{e}_z$ and parameterize \mathbf{n} by spherical variables θ and φ as $\mathbf{n} = \mathbf{e}_x \cos \varphi \sin \theta + \mathbf{e}_y \sin \varphi \sin \theta + \mathbf{e}_z \cos \theta$. If we change \mathbf{m} with keeping $\mathbf{m} \cdot \mathbf{n}$ fixed, it induces only the Berry phase.

To facilitate the following analysis, we examine the symmetric version of the quantum map (44)

$$\begin{aligned}\hat{U} \equiv & \exp \left\{ -i \frac{\mu}{2} \left(\frac{q}{2} + \frac{2-q}{2} \mathbf{m} \cdot \hat{\boldsymbol{\sigma}} \right) \right\} \exp \left\{ -i \lambda \left(\frac{p}{2} + \frac{2-p}{2} \mathbf{n} \cdot \hat{\boldsymbol{\sigma}} \right) \right\} \\ & \times \exp \left\{ -i \frac{\mu}{2} \left(\frac{q}{2} + \frac{2-q}{2} \mathbf{m} \cdot \hat{\boldsymbol{\sigma}} \right) \right\}.\end{aligned}\quad (45)$$

For brevity, we omit the parameters in the following. A possible implementation of the quantum map (45) is available by a periodically driven system that is described by the following Hamiltonian

$$\hat{H}(t) \equiv \mu \left(\frac{q}{2} + \frac{2-q}{2} \mathbf{m} \cdot \hat{\boldsymbol{\sigma}} \right) + \lambda \left(\frac{p}{2} + \frac{2-p}{2} \mathbf{n} \cdot \hat{\boldsymbol{\sigma}} \right) \sum_{j \in \mathbb{Z}} \delta(t - j), \quad (46)$$

where the Floquet operator for a unit time interval $-1/2 \leq t < 1/2$ is \hat{U} . The magnitudes of the magnetic fields of the unperturbed system and the perturbation are

$$\begin{aligned}B_\mu &\equiv \frac{1}{2}(2-q)\mu, \\ B_\lambda &\equiv \frac{1}{2}(2-p)\lambda,\end{aligned}\quad (47)$$

respectively. It is straightforward to show

$$\hat{U} \equiv e^{-i(\mu q + \lambda p)/2} \left(\cos \frac{\Delta}{2} - i \hat{\boldsymbol{\sigma}} \cdot \tilde{\mathbf{l}} \right), \quad (48)$$

where

$$\Delta \equiv 2 \cos^{-1} (\cos B_\mu \cos B_\lambda - \cos \theta \sin B_\mu \sin B_\lambda), \quad (49a)$$

$$\begin{aligned}\tilde{\mathbf{l}} \equiv & (\sin B_\mu \cos B_\lambda + \cos \theta \cos B_\mu \sin B_\lambda) \mathbf{m} \\ & + (\sin B_\lambda) \{ \mathbf{n} - (\mathbf{n} \cdot \mathbf{m}) \mathbf{m} \}.\end{aligned}\quad (49b)$$

It is also easy to see $\|\tilde{\mathbf{l}}\|^2 = \sin^2(\Delta/2)$. Hence $\mathbf{l} \equiv \tilde{\mathbf{l}} / \sin(\Delta/2)$ is a unit vector. Now we have

$$\hat{U} \equiv \exp \left\{ -i \left(\frac{\mu q + \lambda p}{2} + \frac{\Delta}{2} \hat{\boldsymbol{\sigma}} \cdot \mathbf{l} \right) \right\}, \quad (50)$$

and its eigenvalues are

$$z_\pm \equiv \exp \left\{ -i \left(\frac{\mu q + \lambda p}{2} \pm \frac{\Delta}{2} \right) \right\}. \quad (51)$$

Corresponding quasienergies are $E_\pm \equiv (\mu q + \lambda p \pm \Delta)/2$, which is defined up to modulus 2π .

In order to study the adiabatic holonomies, we need to identify the spectral degeneracies, whose condition is $e^{i\Delta} = 1$, in the parameter space. It is useful to see Δ as a function of B_λ

$$\Delta = 2 \cos^{-1} (A \cos(B_\lambda + \tilde{a})) \quad (52)$$

where $A \equiv \sqrt{1 - \sin^2 \theta \sin^2 B_\mu}$ and \tilde{a} is an “initial phase” that is independent with λ . We choose the branch of $\cos^{-1} A$ in $[0, \pi]$. If $A < 1$, Δ oscillates within the range $[2 \cos^{-1} A, 2\pi - 2 \cos^{-1} A] \subset (0, 2\pi)$ as a function of B_λ , and encounters no spectral degeneracy. On the other hand, the condition $A = 1$ (i.e., $\sin \theta \sin B_\mu = 0$) implies the presence of the spectral degeneracy. From the similar argument for B_μ , we will encounter spectral degeneracies if $\sin \theta \sin B_\mu \sin B_\lambda = 0$.

Let us examine the case $\sin \theta = 0$. Since this implies $\cos \theta = \pm 1$, we have

$$\Delta = 2 \cos^{-1} \left(\cos(B_\lambda \pm B_\mu) \right). \quad (53)$$

Accordingly the degeneracy points draw lines in (B_μ, B_λ) -plane as

$$\left\{ (B_\mu, B_\lambda) \mid \frac{B_\lambda \pm B_\mu}{\pi} \in \mathbb{Z} \right\} \quad (54)$$

corresponding to the condition $\cos \theta = \pm 1$. On the other hand, if we assume $\sin B_\mu \sin B_\lambda = 0$, we have

$$\Delta = 2 \cos^{-1} \left(\cos B_\mu \cos B_\lambda \right). \quad (55)$$

Hence another condition for the spectral degeneracy is $|\cos B_\mu \cos B_\lambda| = 1$, i.e., the degeneracy points are at lattice points:

$$\left\{ (B_\mu, B_\lambda) \mid \frac{B_\mu}{\pi}, \frac{B_\lambda}{\pi} \in \mathbb{Z} \right\}, \quad (56)$$

for all θ .

Summarizing above, we show the location of the spectral degeneracies in terms of (μ, ν) , whose space is the two-dimensional torus. The degeneracy lines are specified by (μ, λ, θ) as

$$\left\{ (\mu, \lambda, \theta) \mid \frac{\lambda(2-p) + \mu(2-q) \cos \theta}{2\pi} \in \mathbb{Z}, \frac{\theta}{\pi} \in \mathbb{Z} \right\}. \quad (57)$$

In addition to this, we have isolated degeneracy points as

$$\left\{ \left(\mu = \frac{2\pi k}{2-q}, \lambda = \frac{2\pi l}{2-p} \right) \mid k, l \in \mathbb{Z} \right\}. \quad (58)$$

Except these degeneracy points, it is legitimate to introduce a zenith angle Θ of L , s.t.,

$$\begin{aligned} \cos \Theta &= \frac{\sin B_\mu \cos B_\lambda + \cos \theta \cos B_\mu \sin B_\lambda}{\sin(\Delta/2)}, \\ \sin \Theta &= \frac{\sin \theta \sin B_\lambda}{\sin(\Delta/2)}. \end{aligned} \quad (59)$$

It is straightforward to obtain the eigenvectors $|\xi_\pm\rangle$ of \hat{U} , corresponding to the eigenvalues z_\pm :

$$|\xi_+\rangle = e^{-i\varphi/2} \cos \frac{\Theta}{2} |\uparrow\rangle + e^{i\varphi/2} \sin \frac{\Theta}{2} |\downarrow\rangle, \quad (60a)$$

$$|\xi_-\rangle = -e^{-i\varphi/2} \sin \frac{\Theta}{2} |\uparrow\rangle + e^{i\varphi/2} \cos \frac{\Theta}{2} |\downarrow\rangle. \quad (60b)$$

Let $f \equiv [|\xi_+\rangle, |\xi_-\rangle]$ be a frame. The gauge connections (6) for f are

$$A_\theta = \frac{1}{2}\sigma_y \frac{\partial \Theta}{\partial \theta}, \quad (61a)$$

$$A_\varphi = \frac{1}{2}(\sigma_z \cos \Theta - \sigma_x \sin \Theta), \quad (61b)$$

$$A_\lambda = \frac{1}{2}\sigma_y \frac{\partial \Theta}{\partial \lambda}, \quad (61c)$$

$$A_\mu = \frac{1}{2}\sigma_y \frac{\partial \Theta}{\partial \mu}, \quad (61d)$$

and the corresponding Mead-Truhlar-Berry gauge connections are $A_\theta^D = 0$, $A_\varphi^D = \frac{1}{2}\sigma_z \cos \Theta$, $A_\lambda^D = 0$, and $A_\mu^D = 0$. With these gauge connections, we will examine the holonomy matrices of typical loops in the parameter space.

First, we examine the meridian great circle C_θ in which θ moves 0 to 2π with other parameters are kept fixed. It is straightforward to see $B(C_\theta) = 1$, due to the parallel transport condition $A_\theta^D = 0$. Hence all the holonomies reside in $W(C_\theta) = M(C_\theta)$:

$$\begin{aligned} W(C_\theta) &= \exp \left(-i \oint_{C_\theta} \frac{1}{2} \sigma_y \frac{\partial \Theta}{\partial \theta} d\theta \right) \\ &= \exp \left(-i \frac{1}{2} \sigma_y \Theta|_{\theta=0}^{2\pi} \right), \end{aligned} \quad (62)$$

where $\Theta|_{\theta=0}^{2\pi}$, the change of Θ along C_θ , is determined by the image of C_θ in the sphere (Θ, φ) . If the image is a closed circle, we have $\Theta|_{\theta=0}^{2\pi} = \pm 2\pi$, where \pm correspond to the direction of the path. Both cases provides a Longuet-Higgins type phase change $M(C_\theta) = e^{\mp i\pi\sigma_y} = -1$. On the other hand, if the image is closed self-retracing curve along an ark, we have $\Theta|_{\theta=0}^{2\pi} = 0$, which implies $M(C_\theta) = 1$. The following index

$$r \equiv \left\lfloor \frac{B_\lambda + B_\mu}{\pi} \right\rfloor - \left\lfloor \frac{B_\lambda - B_\mu}{\pi} \right\rfloor, \quad (63)$$

where $[x]$ is the maximum integer not greater than x , determines which is the case, as shown in Appendix B:

$$\Theta|_{\theta=0}^{2\pi} = \begin{cases} 2\pi(-1)^{r/2} & \text{for } r \text{ is even} \\ 0 & \text{for } r \text{ is odd} \end{cases}. \quad (64)$$

Hence we obtain

$$M(C_\theta) = (-1)^{1+r}. \quad (65)$$

Next, we examine a circle of latitude C_φ , where φ is increased from 0 to 2π and the other parameters are kept fixed. We have $B(C_\varphi) = \exp(i\pi\sigma_z \cos \Theta)$ and $W(C_\varphi) = -1$. Accordingly, we obtain

$$M(C_\varphi) = \exp(-i\pi(1 - \cos \Theta)\sigma_z). \quad (66)$$

So far, the holonomy matrices $M(C)$ are diagonal, so that neither C_θ nor C_φ incorporates the exotic holonomies. The following is the first example of the exotic holonomies in this paper.

Let us examine a closed loop C_λ , in which λ is increased from 0 to 2π , being kept fixed other parameters. To avoid degeneracies along C_λ , we choose $\mu(2-q)/(2\pi) \notin \mathbb{Z}$ and $\theta/\pi \notin \mathbb{Z}$. When we increase λ from $\lambda = \lambda'$ to $\lambda = \lambda' + 2\pi$, we have

$$\Delta|_{\lambda=\lambda'+2\pi} = \begin{cases} \Delta|_{\lambda=\lambda'} & \text{for even } p \\ 2\pi - \Delta|_{\lambda=\lambda'} & \text{for odd } p \end{cases}, \quad (67)$$

i.e., an anholonomy in Δ occurs. Accordingly we have an eigenvalue holonomy

$$z_\pm|_{\lambda=\lambda'+2\pi} = \begin{cases} z_\pm|_{\lambda=\lambda'} & \text{for even } p \\ z_\mp|_{\lambda=\lambda'} & \text{for odd } p \end{cases}, \quad (68)$$

which implies the presence of the eigenspace holonomy. We proceed to evaluate the holonomy matrix $M(C_\lambda)$. Because of the parallel transport condition $A_\lambda^D = 0$, we have $M(C_\lambda) = W(C_\lambda)$. On the other hand, we have

$$\begin{aligned} W(C_\lambda) &= \exp\left(-i \oint_{C_\lambda} \frac{1}{2} \sigma_y \frac{\partial \Theta}{\partial \lambda} d\lambda\right) \\ &= \exp\left(-i \frac{1}{2} \sigma_y \Theta|_{\lambda=0}^{\lambda=2\pi}\right). \end{aligned} \quad (69)$$

Hence we need to examine the zenith angle Θ . From Eq. (59) and $\sin(\Delta/2)|_{\lambda=\lambda'+2\pi} = \sin(\Delta/2)|_{\lambda=\lambda'}$, we have $e^{i\Theta}|_{\lambda=2\pi} = (-1)^{(2-p)} e^{i\Theta}|_{\lambda=0}$, i.e., $\Theta|_{\lambda=0}^{2\pi} = \pi(2-p) \bmod 2\pi$. Since this is not suffice to determine the precise value of $W(C_\lambda)$, we need keep track of Θ against the increment of λ to obtain $\Theta|_{\lambda=0}^{2\pi}$. Now the parameter space perpendicular to C_λ is $(\theta, \varphi, \mu) \in S^2 \times S^1$, which is divided into subspaces by the spectral degeneracies $\mu = 2\pi k/(2-q)$ (k is integer). Since, in each subspace, $\Theta|_{\lambda=0}^{2\pi}$ is constant, it is suffice to evaluate it at a representative point. Let us choose a point $\theta = \pi/2$ and $\mu = \pi(2k+1)/(2-q)$, where the spectral gap takes a constant value $\Delta = \pi$, from Eq. (49a). Accordingly we have $e^{i\Theta} = (-1)^k \exp\{i(-1)^k \lambda(2-p)/2\}$, from Eq. (59). Hence we obtain

$$\Theta|_{\lambda=0}^{2\pi} = (-1)^k \pi(2-p), \quad (70)$$

which also holds for $2\pi k/(2-q) < \mu < 2\pi(k+1)/(2-q)$, i.e., $k = [\mu(2-q)/(2\pi)]$. Hence we have

$$\begin{aligned} M(C_\lambda) &= \exp\left(-i \frac{1}{2} (-1)^k \pi(2-p) \sigma_y\right) \\ &= \begin{bmatrix} -\cos \frac{p\pi}{2}, & -(-1)^k \sin \frac{p\pi}{2} \\ (-1)^k \sin \frac{p\pi}{2}, & -\cos \frac{p\pi}{2} \end{bmatrix}. \end{aligned} \quad (71)$$

In particular, if p is odd, the off-diagonal elements of $M(C_\lambda)$ remains, so that the eigenspace holonomy exhibits. This is consistent with the emergence of the eigenvalue holonomy for odd p .

Now the similar analysis of quantum holonomies for the circuit C_μ , where μ is increased from 0 to 2π , is trivial. Hence we show only the holonomy matrix

$$M(C_\mu) = \begin{bmatrix} -\cos \frac{q\pi}{2}, & -(-1)^k \sin \frac{q\pi}{2} \\ (-1)^k \sin \frac{q\pi}{2}, & -\cos \frac{q\pi}{2} \end{bmatrix}, \quad (72)$$

where $k = [\lambda(2-p)/(2\pi)]$. We conclude that odd q along C_μ implies the exotic holonomies.

5. Example 3: the exotic holonomies a la Wilczek-Zee

A simple example of the eigenspace holonomy accompanying spectral degeneracy is shown. Extending Mead's study [16, 17] on non-Abelian adiabatic phase holonomy [6], we introduce a quantum map with Kramer's degeneracy.

5.1. Quantum map for spin- $\frac{3}{2}$ with Kramers' degeneracy

To introduce our model, we review the time-reversal invariance structure in an atom with odd-number of electrons [16, 17]. For a comprehensive explanation, we refer Avron *et al.* [17]. Let $\hat{\mathbf{J}}$ be the total angular momentum of our system and $|J, M\rangle$ the standard basis vector for $\hat{\mathbf{J}}$, i.e., $\hat{\mathbf{J}}^2|J, M\rangle = J(J+1)|J, M\rangle$, $\hat{\mathbf{J}} \cdot \mathbf{e}_z|J, M\rangle = M|J, M\rangle$, and $\hat{\mathbf{J}} \cdot (\mathbf{e}_x \pm i\mathbf{e}_y)|J, M\rangle = \sqrt{J(J+1) - M(M \pm 1)}|J, M \pm 1\rangle$. The standard time-reversal operator for $\hat{\mathbf{J}}$ is an anti-unitary operator $\hat{K} \equiv \exp(-i\pi\hat{J}_y)\hat{K}_0$, where \hat{K}_0 is the complex conjugate operation in the $|J, M\rangle$ -representation. We examine the fermion case $\hat{K}^2 = -1$, which implies that J is a half-integer. If an Hermite operator commutes with \hat{K} , its spectrum exhibits Kramer's degeneracy. The same is true for unitary operators.

We focus on the case $J = \frac{3}{2}$, and introduce basis vectors as follows:

$$\begin{aligned} |e_1\rangle &\equiv |\frac{3}{2}, \frac{3}{2}\rangle, & |Ke_1\rangle &\equiv \hat{K}(|e_1\rangle) = |\frac{3}{2}, -\frac{3}{2}\rangle, \\ |e_2\rangle &\equiv |\frac{3}{2}, -\frac{1}{2}\rangle, & |Ke_2\rangle &\equiv \hat{K}(|e_2\rangle) = |\frac{3}{2}, \frac{1}{2}\rangle. \end{aligned} \quad (73)$$

Our physical observables are spanned by the following time-reversal invariant operators

$$\begin{aligned} \hat{\tau}_0 &\equiv |e_1\rangle\langle e_1| + |Ke_1\rangle\langle Ke_1| - |e_2\rangle\langle e_2| - |Ke_2\rangle\langle Ke_2|, \\ \hat{\tau}_1 &\equiv |e_1\rangle\langle Ke_2| + |Ke_1\rangle\langle e_2| + \text{h.c.}, \\ \hat{\tau}_2 &\equiv |e_1\rangle\langle -i\rangle\langle Ke_2| + |Ke_1\rangle\langle -i\rangle\langle e_2| + \text{h.c.}, \\ \hat{\tau}_3 &\equiv |e_1\rangle\langle e_2| + |Ke_1\rangle\langle Ke_2| + \text{h.c.}, \\ \hat{\tau}_4 &\equiv |e_1\rangle\langle -i\rangle\langle e_2| + |Ke_1\rangle\langle i\rangle\langle Ke_2| + \text{h.c.}, \end{aligned} \quad (74)$$

which are traceless and form a Clifford algebra

$$\hat{\tau}_\alpha \hat{\tau}_\beta + \hat{\tau}_\beta \hat{\tau}_\alpha = 2\delta_{\alpha\beta}. \quad (75)$$

Several properties of τ_α are shown in Appendix C.

We introduce an extension of the quantum map for spin- $\frac{1}{2}$ (Eq. (45))

$$\begin{aligned} \hat{U} &\equiv \exp\left\{-i\frac{\mu}{2}\left(\frac{q}{2} + \frac{2-q}{2}\hat{\tau}_0\right)\right\} \exp\left\{-i\lambda\left(\frac{p}{2} + \frac{2-p}{2}\sum_{\alpha=0}^4 n_\alpha \hat{\tau}_\alpha\right)\right\} \\ &\times \exp\left\{-i\frac{\mu}{2}\left(\frac{q}{2} + \frac{2-q}{2}\hat{\tau}_0\right)\right\}, \end{aligned} \quad (76)$$

where $(n_\alpha)_{\alpha=0}^4$ is a unit vector in \mathbb{R}^5 , i.e., $\sum_\alpha n_\alpha^2 = 1$, and $(q, p) \in \mathbb{Z}^2$. The quantum map (76) can be implemented by a periodically pulsed driven system in a similar way shown in the previous section for the quantum map (45). Since the unitary operator (76) is 2π -periodic both in μ and

λ , the parameter space of (μ, λ) forms a two-dimensional torus $S^1 \times S^1$. The unit vector (n_α) is parameterized by spherical variables:

$$n_0 = \cos \theta, \quad \begin{bmatrix} n_1 \\ n_2 \end{bmatrix} = \begin{bmatrix} \cos \chi \\ \sin \chi \end{bmatrix} \sin \eta \sin \theta, \quad \begin{bmatrix} n_3 \\ n_4 \end{bmatrix} = \begin{bmatrix} \cos \varphi \\ \sin \varphi \end{bmatrix} \cos \eta \sin \theta. \quad (77)$$

In Appendix D, we show

$$\hat{U} = e^{-i(\mu q + \lambda p)/2} \left(\cos \frac{\Delta}{2} - i \sum_{\alpha} \tilde{l}_{\alpha} \hat{\tau}_{\alpha} \right), \quad (78)$$

where Δ is defined in Eq. (49a),

$$\tilde{l}_0 = \sin B_{\mu} \cos B_{\lambda} + \cos \theta \cos B_{\mu} \sin B_{\lambda}, \quad (79a)$$

and

$$\tilde{l}_{\alpha} \equiv n_{\alpha} \sin B_{\lambda} \quad (79b)$$

for $\alpha \neq 0$, where the definitions of B_{μ} and B_{λ} are shown in Eq. (47). Since $\sum_{\alpha=0}^4 \tilde{l}_{\alpha}^2 = \sin^2(\Delta/2)$, we normalize \tilde{l}_{α} :

$$l_{\alpha} \equiv \frac{1}{\sin(\Delta/2)} \tilde{l}_{\alpha}. \quad (80)$$

Accordingly we have

$$\hat{U} = \exp \left\{ -i \left(\frac{\mu q + \lambda p}{2} + \frac{\Delta}{2} \sum_{\alpha} l_{\alpha} \hat{\tau}_{\alpha} \right) \right\}. \quad (81)$$

The eigenvalues of \hat{U} are

$$z_{\pm} \equiv \exp \left\{ -i \left(\frac{\mu q + \lambda p}{2} \pm \frac{\Delta}{2} \right) \right\}. \quad (82)$$

Namely, the spectrum is completely same with the example shown in Section 4. To examine eigenvectors, we parametrize l_{α} with the zenith angle Θ , which is already introduced for the quantum map spin- $\frac{1}{2}$ in Eq. (59). We have

$$l_0 = \cos \Theta, \quad \begin{bmatrix} l_1 \\ l_2 \end{bmatrix} = \begin{bmatrix} \cos \chi \\ \sin \chi \end{bmatrix} \sin \eta \sin \Theta, \quad \begin{bmatrix} l_3 \\ l_4 \end{bmatrix} = \begin{bmatrix} \cos \varphi \\ \sin \varphi \end{bmatrix} \cos \eta \sin \Theta. \quad (83)$$

From Appendix E, the eigenvectors of \hat{U} are

$$\begin{aligned} |\xi_{+}\rangle &= |d_1\rangle \cos \frac{\Theta}{2} + |d_2\rangle \sin \frac{\Theta}{2}, \\ |K\xi_{+}\rangle &= |Kd_1\rangle \cos \frac{\Theta}{2} + |Kd_2\rangle \sin \frac{\Theta}{2}, \\ |\xi_{-}\rangle &= |d_1\rangle \left(-\sin \frac{\Theta}{2} \right) + |d_2\rangle \cos \frac{\Theta}{2}, \\ |K\xi_{-}\rangle &= |Kd_1\rangle \left(-\cos \frac{\Theta}{2} \right) + |Kd_2\rangle \sin \frac{\Theta}{2}, \end{aligned} \quad (84)$$

where

$$\begin{aligned}
|d_1\rangle &\equiv |e_1\rangle \left(e^{-i(\varphi+\chi)/2} \cos \frac{\eta}{2} \right) + |Ke_1\rangle \left(-e^{+i(\varphi+\chi)/2} \sin \frac{\eta}{2} \right), \\
|d_2\rangle &\equiv |e_2\rangle \left(e^{i(\varphi-\chi)/2} \cos \frac{\eta}{2} \right) + |Ke_2\rangle \left(e^{-i(\varphi-\chi)/2} \sin \frac{\eta}{2} \right), \\
|Kd_1\rangle &= |e_1\rangle \left(+e^{-i(\varphi+\chi)/2} \sin \frac{\eta}{2} \right) + |Ke_1\rangle \left(e^{+i(\varphi+\chi)/2} \cos \frac{\eta}{2} \right), \\
|Kd_2\rangle &= |e_2\rangle \left(-e^{+i(\varphi-\chi)/2} \sin \frac{\eta}{2} \right) + |Ke_2\rangle \left(e^{-i(\varphi-\chi)/2} \cos \frac{\eta}{2} \right).
\end{aligned} \tag{85}$$

Note that we put each basis vector before its complex coefficient above to prevent a confusion due to the presence of anti-Hermite operation K . To conclude this subsection, we introduce a frame composed by the eigenvectors \hat{U} [18]:

$$f \equiv [|\xi_+\rangle, |K\xi_+\rangle, |\xi_-\rangle, |K\xi_-\rangle]. \tag{86}$$

5.2. Analysis of adiabatic holonomies

We examine the adiabatic holonomies of the quantum map. Note that Δ and Θ depend only on μ, λ, θ and is the same ones for the quantum map spin-1/2 (see, Eqs. (45), and (59)). Hence the degeneracy points in the parameter space and the holonomy in the eigenvalues are the completely the same. We will focus on the eigenspace holonomy in the following.

It is straightforward to obtain the gauge connection from the eigenvectors. Since Θ depends on μ, λ, θ , the corresponding gauge connections are defined through the derivative of f by Θ :

$$A_x = if^\dagger \frac{\partial}{\partial x} f = \frac{1}{2} \begin{bmatrix} 0 & -iI_2 \\ +iI_2 & 0 \end{bmatrix} \frac{\partial \Theta}{\partial x}, \tag{87}$$

for $x = \theta, \mu, \lambda$, where I_2 is the 2×2 unit matrix. The corresponding Wilczek-Zee gauge connections vanish to satisfy the parallel transport condition, i.e.. $A_\theta^D = A_\mu^D = A_\lambda^D = 0$. For other gauge connections, μ, λ , and θ -dependences are introduced through Θ :

$$A_\eta = \frac{1}{2} \begin{bmatrix} -\sigma_y \cos \Theta & \sigma_y \sin \Theta \\ \sigma_y \sin \Theta & \sigma_y \cos \Theta \end{bmatrix}, \tag{88a}$$

$$A_\varphi = \frac{1}{2} \begin{bmatrix} \sigma_z \cos \Theta & -\sigma_z \sin \Theta \\ -\sigma_z \sin \Theta & -\sigma_z \cos \Theta \end{bmatrix} \cos \eta + \frac{1}{2} \begin{bmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{bmatrix} \sin \eta, \tag{88b}$$

$$A_\chi = \frac{1}{2} \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix} \cos \eta + \frac{1}{2} \begin{bmatrix} \sigma_x \cos \Theta & -\sigma_x \sin \Theta \\ -\sigma_x \sin \Theta & -\sigma_x \cos \Theta \end{bmatrix} \sin \eta, \tag{88c}$$

and

$$A_\eta^D = \frac{1}{2} \begin{bmatrix} -\sigma_y & 0 \\ 0 & \sigma_y \end{bmatrix} \cos \Theta, \tag{89a}$$

$$A_\varphi^D = \frac{1}{2} \begin{bmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{bmatrix} \cos \Theta \cos \eta + \frac{1}{2} \begin{bmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{bmatrix} \sin \eta, \tag{89b}$$

$$A_\chi^D = \frac{1}{2} \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix} \cos \eta + \frac{1}{2} \begin{bmatrix} \sigma_x & 0 \\ 0 & -\sigma_x \end{bmatrix} \cos \Theta \sin \eta. \tag{89c}$$

It is straightforward to evaluate the holonomy matrix $M(C_\alpha)$ (25) for a closed loop C_α where $\alpha(=\mu, \lambda, \theta, \eta, \varphi, \chi)$ is increased from 0 to 2π , once we take care the “anholonomy” in Θ along C_α , which is also clarified in Section 4. For μ, λ, θ , we have

$$\begin{aligned} M(C_\alpha) &= \exp\left(-\frac{i}{2} \begin{bmatrix} 0 & -iI_2 \\ +iI_2 & 0 \end{bmatrix} \Theta|_{\alpha=0}^{2\pi}\right) \\ &= \begin{bmatrix} I_2 \cos \frac{\Theta|_{\alpha=0}^{2\pi}}{2} & -I_2 \sin \frac{\Theta|_{\alpha=0}^{2\pi}}{2} \\ +I_2 \sin \frac{\Theta|_{\alpha=0}^{2\pi}}{2} & I_2 \cos \frac{\Theta|_{\alpha=0}^{2\pi}}{2} \end{bmatrix}, \end{aligned} \quad (90)$$

where

$$\Theta|_{\theta=0}^{2\pi} = \begin{cases} 2\pi(-1)^{r/2} & \text{for } r \text{ is even} \\ 0 & \text{for } r \text{ is odd} \end{cases}, \quad (91a)$$

$$\Theta|_{\lambda=0}^{2\pi} = (-1)^{[\mu(2-q)/(2\pi)]} \pi(2-p), \quad (91b)$$

$$\Theta|_{\mu=0}^{2\pi} = (-1)^{[\lambda(2-p)/(2\pi)]} \pi(2-q), \quad (91c)$$

and r is defined in Eq. (63). Hence $M(C_\theta)$ exhibits only Herzberg and Longuet-Higgins’ sign change [15]

$$M(C_\theta) = (-1)^{1+r} I_4. \quad (92)$$

Also, the same kind of sign change appears along C_μ (C_λ) with even p (q), i.e., $M(C_\mu) = (-1)^{1+p/2} I_4$ ($M(C_\lambda) = (-1)^{1+q/2} I_4$). On the other hand, a mixture of the eigenspace holonomy and the Herzberg and Longuet-Higgins’ sign change occurs along C_μ with odd p

$$M(C_\mu) = (-1)^{[\mu(2-q)/(2\pi)]+(p-1)/2} \begin{bmatrix} 0 & -I_2 \\ I_2 & 0 \end{bmatrix}, \quad (93)$$

and, along C_λ with odd q

$$M(C_\lambda) = (-1)^{[\lambda(2-p)/(2\pi)]+(q-1)/2} \begin{bmatrix} 0 & -I_2 \\ I_2 & 0 \end{bmatrix}, \quad (94)$$

which do not incorporate mixing within the degenerate eigenspaces. Other holonomy matrices $M(C_\alpha)$ ($\alpha = \eta, \varphi, \chi$) describes genuine Wilczek-Zee’s phase holonomies:

$$M(C_\eta) = \begin{bmatrix} \exp(i\sigma_y \Omega_\eta/2) & 0 \\ 0 & \exp(-i\sigma_y \Omega_\eta/2) \end{bmatrix}, \quad (95a)$$

$$M(C_\varphi) = \begin{bmatrix} \exp[-i(\sigma_z \cos \eta_1 + \sigma_x \sin \eta_1) \Omega_1/2] & 0 \\ 0 & \exp[i(\sigma_z \cos \eta_1 - \sigma_x \sin \eta_1) \Omega_1/2] \end{bmatrix}, \quad (95b)$$

$$M(C_\chi) = \begin{bmatrix} \exp[-i(\sigma_z \cos \eta_2 + \sigma_x \sin \eta_2) \Omega_2/2] & 0 \\ 0 & \exp[-i(\sigma_z \cos \eta_2 - \sigma_x \sin \eta_2) \Omega_2/2] \end{bmatrix}, \quad (95c)$$

where $\Omega_\eta \equiv 2\pi(1 - \cos \Theta)$, $\Omega_j \equiv 2\pi(1 - \beta_j)$, $\eta_j \equiv -i \ln \{(\cos \Theta \cos \eta + i \sin \eta)/\beta_j\}$ for $j = 1, 2$, $\beta_1 \equiv \sqrt{1 - (\sin \Theta \cos \eta)^2}$ and $\beta_2 \equiv \sqrt{1 - (\sin \Theta \sin \eta)^2}$.

6. Summary and outlook

We have introduced a framework that is capable of describing the eigenspace holonomy and the phase holonomy in a unified manner. Several examples have been shown.

In hindsight, it might seem rather odd that, in two decades since the first discovery of Berry phase, the full, gauge invariant formulation for quantum holonomy has not been conceived prior to this work. It should probably be attributed to the lack of the incentive to improve on the original expression of Berry; Nothing other than the phase anholonomy has been anticipated for the adiabatic cyclic variation of parameters for regular Hamiltonian system. As a result, the gauge invariant formulation must have seemed a redundant luxury. However, if we once recognize the possibility of eigenstates' exchange without level crossing for cyclic parameter variation, both for singular systems and for time-periodic systems, it becomes imperative to treat the choice of basis frame explicitly within the formalism, which has naturally lead us to arrive at the full, gauge invariant formulae.

In a simple minded view, it is the periodicity of quasienergy, which is a result of the time-periodicity of the system, that enables the eigenvalue holonomy in a natural manner. For a Hamiltonian system, with the energy defined on entire real number, an energy eigenstate after cyclic variation of parameter cannot reach another eigenstate of different energy in a usual way, since the crossing of levels is prohibited for adiabatic variation. The only possible exception appears to be *singular* Hamiltonian systems, for which the highest and the ground eigenenergy diverge [4].

In this work, we have focused on the most elementary setting of quantum holonomy, *i.e.*, the adiabatic excursion of pure quantum eigenstates along a closed path in the parameter space. A vast amount of studies on the phase holonomy naturally suggests possible directions of extension of the present result. We mention only few of them. A straightforward extension is to examine noncyclic path [19, 12]. Also, loosening of the assumption of adiabaticity and resulting extension into *e.g.* Aharonov-Anandan's nonadiabatic settings [20], are expected to be straightforward thanks to the generality of Fujikawa's formulation [9], which is the basis of our theory. It seems timely as well as interesting to examine the eigenspace holonomy in dissipative systems, for which we will need to horn appropriate techniques to treat of the eigenspace holonomy in mixed states [21].

Finally, we mention a question that is raised from the main result Eq. (25), which supplies a complete prescription to quantify the adiabatic quantum holonomy. How this helps to understand the exotic holonomies intuitively? Is it possible to find any underlying object or concept that governs them, for example, in the manner of diabolic point for the case of Berry phase? Herzberg and Longuet-Higgins has shown that the phase holonomy along a closed loop C implies the presence of spectral degeneracy in a surface S enclosed by C in the parameter space [15] (see also, Refs. [10, 22]). Is there any counterpart of the argument of Herzberg and Longuet-Higgins for the exotic holonomies? This does not seem likely, for the case of exotic holonomy, at the first glance, since there is no room to make S from C in all the examples shown in this paper. We now believe that an affirmative answer is to be found in the *complex parameter plane*, on which we shall focus our attention in a forthcoming publication.

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A. The gauge theory for Hamiltonian time evolution

We will derive the holonomy matrix (Eq. (25)) for a system described by Hamiltonian $\hat{H}(s)$ that depends on a time-dependent parameter s . Suppose that s is moved from s' to s'' along a path C , during $0 \leq t \leq T$. The corresponding time evolution operator is

$$\hat{U}(\{s_t\}_{t \in [0, T]}) \equiv \exp_{\leftarrow} \left(-\frac{i}{\hbar} \int_0^T \hat{H}(s_t) dt \right). \quad (96)$$

We divide the time interval $[0, T]$ into L parts. Let $t_l \equiv (l/L)T$. A short time evolution operator \hat{U}_l is accordingly introduced:

$$\hat{U}_l \equiv \exp_{\leftarrow} \left(-\frac{i}{\hbar} \int_{t_l}^{t_{l+1}} \hat{H}(s_t) dt \right). \quad (97)$$

When L is large enough, we have

$$\hat{U}_l = \exp \left(-\frac{i}{\hbar} \hat{H}(s_l) \epsilon \right) + \mathcal{O}(\epsilon^2), \quad (98)$$

where $s_l \equiv \frac{1}{2}(s_{t_{l+1}} + s_{t_l})$ and $\epsilon \equiv T/L$. Now we introduce a s -dependent unitary operator

$$\hat{U}_s \equiv \exp \left(-\frac{i}{\hbar} \hat{H}(s) \epsilon \right). \quad (99)$$

Accordingly we have

$$\hat{U}(\{s_t\}_{t \in [0, T]}) = \prod_{\leftarrow, l=0}^{L-1} \hat{U}_{s_l} + \mathcal{O}(\epsilon). \quad (100)$$

Since we choose L so as to satisfy $\epsilon \ll 1$, our formulation explained in Section 2 is straightforwardly applicable.

First, for a given $f(s)$, the $f(s)$ -representation of $U(s)$ is

$$Z(s) = \exp \left(-\frac{i}{\hbar} \{f(s)^\dagger\} \hat{H}(s) f(s) \epsilon \right) + \mathcal{O}(\epsilon^2). \quad (101)$$

On the other hand, we have

$$\exp_{\leftarrow} \left(i \int_{s_l}^{s_{l+1}} A(s) ds \right) = \exp(iA(s_l) \dot{s} \epsilon) + \mathcal{O}(\epsilon^2), \quad (102)$$

where we assumed $\dot{s} = \mathcal{O}(1)$. Hence we have

$$\exp_{\leftarrow} \left(i \int_{s_l}^{s_{l+1}} A(s) ds \right) Z(s_l) = \exp \left(-\frac{i}{\hbar} F(s_l, \dot{s}) \epsilon \right) + \mathcal{O}(\epsilon^2), \quad (103)$$

where we introduce Fujikawa's Hamiltonian matrix [9]

$$F(s, \dot{s}) \equiv \{f(s)^\dagger\} \hat{H}(s) f(s) - \hbar A(s) \dot{s}. \quad (104)$$

In the limit $L \rightarrow \infty$, the effective time evolution operator for Fujikawa's formulation [9] is

$$B_d(\{s_t\}) = \exp\left(-\frac{i}{\hbar} \int_0^T F(s_t, \dot{s}_t) dt\right). \quad (105)$$

Next, let us examine the adiabatic change of s . Let $f(s)$ be an adiabatic basis for $\hat{H}(s)$. Now

$$H^D(s) \equiv f(s)^\dagger \hat{H}(s) f(s) \quad (106)$$

is a diagonal matrix whose non-zero elements are the eigenvalues of $\hat{H}(s)$. Thanks to the adiabatic theorem, we employ the diagonal approximation for $B_d(\{s_t\})$:

$$B_d(\{s_t\}) \simeq B_{ad}(\{s_t\}) \equiv \exp\left(-\frac{i}{\hbar} \int_0^T F^D(s, \dot{s}) dt\right), \quad (107)$$

where $F^D(s, \dot{s})$ is defined as

$$F^D(s, \dot{s}) \equiv H^D(s) - \hbar A^D(s) \dot{s}. \quad (108)$$

Hence $B_{ad}(\{s_t\})$ is decomposed into geometric and dynamical factors:

$$B_{ad}(\{s_t\}) = \exp\left(i \int_{s'}^{s''} A^D(s) ds\right) \exp\left(-\frac{i}{\hbar} \int_0^T H^D(s) dt\right). \quad (109)$$

Now it is trivial to apply our formulation explained in the main text to obtain the holonomy matrix (Eq. (25)).

B. A derivation of Eq. (65)

To evaluate Eq. (62), we need to obtain the image of C_θ in the sphere (Θ, φ) . First, we remind that Θ is a periodic function of θ from Eqs. (49a) and (59). Hence $\Theta|_{\theta=0}^{2\pi}$ must be a multiple of 2π . Second, we remind that there is no spectrum degeneracy along the path C_θ if $r_\pm \notin \mathbb{Z}$, where $r_\pm \equiv \{\lambda(2-p) \pm \mu(2-q)\}/(2\pi)$. Namely, the nondegenerate regions are divided into squares by the lattice $(r_+, r_-) \in \mathbb{Z}^2$. Within each square, $\Theta|_{\theta=0}^{2\pi}$ takes a constant value. Accordingly, it is suffice to evaluate them at representative points of the squares.

Let us examine the case $(r_+ - r_-)/2$ is an integer k , which implies $\Delta = 2 \cos^{-1}((-1)^k \cos(\pi(r_+ + r_-)/2))$, $\cos \Theta = (-1)^k \cos \theta \sin(\pi(r_+ + r_-)/2) / \sin(\Delta/2)$, and $\sin \Theta = \sin \theta \sin(\pi(r_+ + r_-)/2) / \sin(\Delta/2)$. Accordingly we have

$$e^{i\Theta} = (-1)^{[k+(r_++r_-)/2]} \exp\{i(-1)^k \theta\}, \quad (110)$$

which implies the image of C_θ is also a great meridian loop in the sphere (Θ, φ) . Thus we have

$$\Theta|_{\theta=0}^{2\pi} = (-1)^k 2\pi. \quad (111)$$

This result is also valid for the case that $([r_+] - [r_-])/2$ is an integer k .

Let us examine the case $(r_+ + r_-)/2$ is an integer l , which implies $\Delta = 2 \cos^{-1}((-1)^l \cos(\pi(r_+ - r_-)/2))$, $\cos \Theta = (-1)^{l+[r_+-r_-]/2}$ and $\sin \Theta = 0$. Namely, the image of C_θ is a point in (Θ, φ) space. Accordingly we have

$$\Theta|_{\theta=0}^{2\pi} = 0. \quad (112)$$

This result is also valid for the case that $[r_+] - [r_-]$ is an odd integer.

To summarize the argument above, we have, from Eq. (62),

$$M(C_\theta) = \exp \{i\pi (1 + [r_+] - [r_-])\}, \quad (113)$$

which is equivalent with Eq. (65).

C. Algebraic properties of $\hat{\tau}_\alpha$

We summarize the algebraic properties of $\hat{\tau}_\alpha$. Details are found in, for example, Ref. [17]. It is straightforward to show that they form a Clifford algebra (75), which implies the following formulas:

$$\hat{\tau}_\alpha \hat{\tau}_\beta \hat{\tau}_\alpha = 2\delta_{\alpha\beta} \hat{\tau}_\alpha - \hat{\tau}_\beta. \quad (114)$$

For $B_\alpha \in \mathbb{R}$,

$$\left(\sum_\alpha B_\alpha \hat{\tau}_\alpha \right)^2 = \|B\|^2, \quad (115)$$

where $\|B\|$ is a norm of real vector, i.e. $\|B\| = \sqrt{\sum_\alpha B_\alpha^2}$. Furthermore, for a real unit vector n that satisfies $\|n\| = 1$,

$$\exp \left(-i\lambda \sum_\alpha n_\alpha \hat{\tau}_\alpha \right) = \cos \lambda - i \left(\sum_\alpha n_\alpha \hat{\tau}_\alpha \right) \sin \lambda, \quad (116)$$

which is 2π -periodic in λ . Next formula is useful to investigate quantum maps:

$$\begin{aligned} & \exp(-i\lambda \hat{\tau}_\alpha) \hat{\tau}_\beta \exp(-i\lambda \hat{\tau}_\alpha) \\ &= (1 - \delta_{\alpha\beta}) \hat{\tau}_\beta + \delta_{\alpha\beta} \{ \cos(2\lambda) \hat{\tau}_\beta - i \sin(2\lambda) \}. \end{aligned} \quad (117)$$

Finally, we show a representation of $\hat{\tau}_\alpha$ by complex 4×4 matrices τ_α in terms of complex 2×2 matrices defined in Eq. (37), i.e., $\hat{\tau}_\alpha = f_0 \tau_\alpha f_0^\dagger$, where $f_0 \equiv [|e_1\rangle, |Ke_1\rangle, |e_2\rangle, |Ke_2\rangle]$:

$$\begin{aligned} \tau_0 &= \begin{bmatrix} I_2 & 0 \\ 0 & -I_2 \end{bmatrix}, \quad \tau_1 = \begin{bmatrix} 0 & i\sigma_y \\ -i\sigma_y & 0 \end{bmatrix}, \quad \tau_2 = \begin{bmatrix} 0 & -i\sigma_x \\ i\sigma_x & 0 \end{bmatrix}, \\ \tau_3 &= \begin{bmatrix} 0 & I_2 \\ I_2 & 0 \end{bmatrix}, \quad \tau_4 = \begin{bmatrix} 0 & -i\sigma_z \\ i\sigma_z & 0 \end{bmatrix}. \end{aligned} \quad (118)$$

D. A derivation of Eq. (78)

We derive Eq. (78) from Eq. (76). First, let $B_\mu \equiv \mu(2 - q)/2$ and $B_\lambda \equiv \lambda(2 - p)/2$. Hence we have

$$\begin{aligned} \hat{U} &= e^{-i(\mu q + \lambda p)/2} e^{-iB_\mu \hat{\tau}_0/2} e^{-iB_\lambda \sum_\alpha n_\alpha \hat{\tau}_\alpha} e^{-iB_\mu \hat{\tau}_0/2}, \\ &= e^{-i(\mu q + \lambda p)/2} e^{-iB_\mu \hat{\tau}_0} \left(\cos B_\lambda - i \sum_\alpha n_\alpha e^{-iB_\mu \hat{\tau}_0/2} \hat{\tau}_\alpha e^{-iB_\mu \hat{\tau}_0/2} \sin B_\lambda \right), \\ &= e^{-i(\mu q + \lambda p)/2} \left(k - i \sum_{\alpha \neq 0} \tilde{l}_\alpha \hat{\tau}_\alpha \right), \end{aligned} \quad (119)$$

where we used Eq. (117) above, and,

$$\begin{aligned} k &\equiv \cos B_\mu \cos B_\lambda - n_0 \sin B_\mu \sin B_\lambda, \\ \tilde{l}_0 &\equiv \sin B_\mu \cos B_\lambda + n_0 \cos B_\mu \sin B_\lambda, \\ \tilde{l}_{\alpha(\neq 0)} &\equiv n_\alpha \sin B_\lambda. \end{aligned} \quad (120)$$

Hence we arrive Eq. (78).

E. Diagonalization of $\sum_\alpha n_\alpha \hat{\tau}_\alpha$

Let n_α ($\alpha = 0, \dots, 4$) be real, and, normalized, i.e. $\sum_{\alpha=0}^4 n_\alpha^2 = 1$. We will obtain the eigenvectors of

$$\hat{\tau}(\{n_\alpha\}) \equiv \sum_{\alpha=0}^4 n_\alpha \hat{\tau}_\alpha, \quad (121)$$

with the help of the quaternionic structure of the Hilbert space induced by the fermion time reversal invariance [17]. We follow the convention of quaternions explained in Ref [17], e.g., $i^2 = j^2 = k^2 = -1$, $ij = -ji = k$, $jk = -kj = i$, and $ki = -ik = j$.

In the Hilbert space \mathcal{H} of spin- $\frac{3}{2}$, we employ a right quaternionic action for $|\psi\rangle \in \mathcal{H}$: $|\psi\rangle i \equiv i|\psi\rangle$, and, $|\psi\rangle j \equiv \hat{K}(|\psi\rangle)$, which implies $|\psi\rangle k = |\psi\rangle(ij) = (|\psi\rangle i)j = \hat{K}(|\psi\rangle i) = -i\{\hat{K}(|\psi\rangle)\}$. Accordingly, for $z_j, w_j \in \mathbb{C}$, we have

$$\begin{aligned} |\psi\rangle &= z_1|e_1\rangle + w_1|Ke_1\rangle + z_2|e_2\rangle + w_2|Ke_2\rangle \\ &= |e_1\rangle(z_1 + jw_1) + |e_2\rangle(z_2 + jw_2) \\ &= f_q \begin{bmatrix} z_1 + jw_1 \\ z_2 + jw_2 \end{bmatrix}, \end{aligned} \quad (122)$$

where

$$f_q \equiv \begin{bmatrix} |e_1\rangle, & |e_2\rangle \end{bmatrix} \quad (123)$$

is the standard frame of the quaternionic Hilbert space. Hence we obtain a natural correspondence between four-dimensional complex vector space and two-dimensional quaternionic vector space. This induces a representation of $\hat{\tau}_\alpha$ by 2×2 quaternionic matrix τ_α^q , i.e.,

$$\hat{\tau}_\alpha = f_q \tau_\alpha^q f_q^\dagger, \quad (124)$$

where

$$\begin{aligned} \tau_0^q &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \tau_1^q \equiv \begin{bmatrix} 0 & -j \\ j & 0 \end{bmatrix}, \quad \tau_2^q \equiv \begin{bmatrix} 0 & k \\ -k & 0 \end{bmatrix}, \\ \tau_3^q &\equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \tau_4^q \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}. \end{aligned} \quad (125)$$

We introduce spherical variables θ, η, χ and φ to parameterize n_α as $n_0 = \cos \theta$, $n_1 = \cos \chi \sin \eta \sin \theta$, $n_2 = \sin \chi \sin \eta \sin \theta$, $n_3 = \cos \varphi \cos \eta \sin \theta$, and $n_4 = \sin \varphi \cos \eta \sin \theta$. In terms of 2×2 quaternionic matrix, we have

$$\hat{\tau}(\{n_\alpha\}) = f_q \begin{bmatrix} \cos \theta & (\cos \eta - j e^{i(\varphi+\chi)} \sin \eta) e^{-i\varphi} \sin \theta \\ e^{+i\varphi} (\cos \eta + j e^{i(\varphi+\chi)} \sin \eta) \sin \theta & -\cos \theta \end{bmatrix} f_q^\dagger, \quad (126)$$

where we introduce

$$h \equiv j e^{i(\varphi+\chi)}. \quad (127)$$

Since $h^2 = j e^{i(\varphi+\chi)} e^{-i(\varphi+\chi)} j = -1$, we have $e^{h\eta} = \cos \eta + h \sin \eta$. Hence we have

$$\hat{\tau}(\{n_\alpha\}) = f_q \begin{bmatrix} \cos \theta & e^{-h\eta} e^{-i\varphi} \sin \theta \\ e^{+i\varphi} e^{h\eta} \sin \theta & -\cos \theta \end{bmatrix} f_q^\dagger. \quad (128)$$

Now it is straightforward to see the eigenvalues of $\hat{\tau}(\{n_\alpha\})$ are ± 1 . Let $|\xi_\pm^{(0)}\rangle$ be corresponding eigenvectors:

$$|\xi_+^{(0)}\rangle \equiv f_q \begin{bmatrix} e^{-h\eta/2} \cos \frac{\theta}{2} \\ e^{i\varphi} e^{h\eta/2} \sin \frac{\theta}{2} \end{bmatrix}, \quad (129a)$$

$$|\xi_-^{(0)}\rangle \equiv f_q \begin{bmatrix} e^{-h\eta/2} \left(-\sin \frac{\theta}{2}\right) \\ e^{i\varphi} e^{h\eta/2} \cos \frac{\theta}{2} \end{bmatrix}. \quad (129b)$$

Instead of the two above, we put a phase factor on them in the following:

$$|\xi_\pm\rangle \equiv |\xi_\pm^{(0)}\rangle e^{-i(\varphi+\chi)/2}, \quad (130)$$

where we need to take care about the noncommutativity of multiplication in quaternions. In the complex Hilbert space, $|\xi_\pm\rangle$ are expressed as

$$|\xi_+\rangle = |d_1\rangle \cos \frac{\theta}{2} + |d_2\rangle \sin \frac{\theta}{2}, \quad (131a)$$

$$|\xi_-\rangle = |d_1\rangle \left(-\sin \frac{\theta}{2}\right) + |d_2\rangle \cos \frac{\theta}{2}, \quad (131b)$$

where $|d_1\rangle$ and $|d_2\rangle$ are orthonormal

$$|d_1\rangle \equiv |e_1\rangle \left(e^{-i(\varphi+\chi)/2} \cos \frac{\eta}{2}\right) + |Ke_1\rangle \left(-e^{+i(\varphi+\chi)/2} \sin \frac{\eta}{2}\right), \quad (132a)$$

$$|d_2\rangle \equiv |e_2\rangle \left(e^{i(\varphi-\chi)/2} \cos \frac{\eta}{2}\right) + |Ke_2\rangle \left(e^{-i(\varphi-\chi)/2} \sin \frac{\eta}{2}\right). \quad (132b)$$

We explain the rest of eigenvectors of $\hat{\tau}(\{n_\alpha\})$ for the complex Hilbert space. They are obtained by the time-reversal operation on $|\xi_\pm\rangle$:

$$|K\xi_+\rangle = |Kd_1\rangle \cos \frac{\theta}{2} + |Kd_2\rangle \sin \frac{\theta}{2}, \quad (133a)$$

$$|K\xi_-\rangle = |Kd_1\rangle \left(-\cos \frac{\theta}{2}\right) + |Kd_2\rangle \cos \frac{\theta}{2}, \quad (133b)$$

where

$$|Kd_1\rangle = |e_1\rangle \left(+e^{-i(\varphi+\chi)/2} \sin \frac{\eta}{2}\right) + |Ke_1\rangle \left(e^{+i(\varphi+\chi)/2} \cos \frac{\eta}{2}\right), \quad (134a)$$

$$|Kd_2\rangle = |e_2\rangle \left(-e^{+i(\varphi-\chi)/2} \sin \frac{\eta}{2}\right) + |Ke_2\rangle \left(e^{-i(\varphi-\chi)/2} \cos \frac{\eta}{2}\right). \quad (134b)$$

Because of $\hat{K}^2 = -1$, $\{|\xi_\pm\rangle, |K\xi_\pm\rangle\}$ is a complete orthogonal system for \mathcal{H} .

To compute gauge connections for $\{|\xi_{\pm}\rangle, |K\xi_{\pm}\rangle\}$, it is useful to summarize the basis transformation between

$$f \equiv \left[|\xi_+\rangle, |K\xi_+\rangle, |\xi_-\rangle, |K\xi_-\rangle \right], \quad (135a)$$

and

$$f_0 \equiv \left[|e_1\rangle, |Ke_1\rangle, |e_2\rangle, |Ke_2\rangle \right]. \quad (135b)$$

It is straightforward to obtain the following

$$f = f_0 \exp\left(-\frac{i}{2}g_4\chi\right) \exp\left(-\frac{i}{2}g_3\varphi\right) \exp\left(-\frac{i}{2}g_2\eta\right) \exp\left(-\frac{i}{2}g_1\theta\right) \quad (136)$$

where g_α are 4×4 Hermite matrices

$$g_1 \equiv \begin{bmatrix} 0 & -iI_2 \\ iI_2 & 0 \end{bmatrix}, \quad g_2 \equiv \begin{bmatrix} -\sigma_y & 0 \\ 0 & \sigma_y \end{bmatrix}, \quad g_3 \equiv \begin{bmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{bmatrix}, \quad g_4 \equiv \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix}. \quad (137)$$

It is also useful to express g_α in terms of τ_α : $g_1 = -i\tau_0\tau_3$, $g_2 = i\tau_1\tau_3$, $g_3 = -i\tau_3\tau_4$, and $g_4 = -i\tau_1\tau_2$.

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